

Benzamide, 2-methyl-N-undecyl-

Inchi:	InChI=1S/C19H31NO/c1-3-4-5-6-7-8-9-10-13-16-20-19(21)18-15-12-11-14-17(18)2/h11-
InchiKey:	VYAIYGHYALELA-UHFFFAOYSA-N
Formula:	C19H31NO
SMILES:	CCCCCCCCCCCN=C(O)c1ccccc1C
Mol. weight [g/mol]:	289.46

Physical Properties

Property code	Value	Unit	Source
hf	-290.23	kJ/mol	Joback Method
hvap	80.90	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.830		Crippen Method
mcpvol	266.360	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	834.52	K	Joback Method
tc	1032.53	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407403&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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